

Probability of Boundary Condition in Quantum Cosmology

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(Dated: January 20, 2017)

Abstract

One of the main interest in quantum cosmology is to determine boundary conditions for the wave function of the universe which can predict observational data of our universe. For this purpose, we solve the Wheeler-DeWitt equation for a closed universe with a scalar field numerically and evaluate probabilities for boundary conditions of the wave function of the universe. To impose boundary conditions of the wave function, we use exact solutions of the Wheeler-DeWitt equation with a constant scalar field potential. These exact solutions include wave functions with well known boundary condition proposals, the no-boundary proposal and the tunneling proposal. We specify the exact solutions by introducing two real parameters to discriminate boundary conditions, and obtain the probability for these parameters under the requirement of sufficient e-foldings of the inflation. The probability distribution of boundary conditions prefers the tunneling boundary condition to the no-boundary boundary condition. Furthermore, for large values of a model parameter related to the inflaton mass and the cosmological constant, the probability of boundary conditions selects an unique boundary condition different from the tunneling type.

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I. INTRODUCTION

Investigation of the very early period of the universe requires quantum treatment of gravity [1]. However, because we do not have the complete theory of quantum gravity yet in hand, simplified models with reduced dynamical degrees of freedom have been investigated to understand nature of canonical quantum gravity. This approach is the mini-superspace quantum cosmology (a general review of quantum cosmology is given by [2]). A quantum state of the model is represented by the wave function of the universe, which satisfies the Wheeler-DeWitt (WD) equation derived from the procedure of canonical quantization [3]. The wave function of the universe is represented as the path integral by summing over histories of the universe [4].

To obtain the wave function of the universe, we must impose boundary conditions of the WD equation. In the context of the quantum cosmology, there are two major candidates for the boundary condition, the tunneling proposal by Vilenkin [5, 6] and the no-boundary boundary condition proposal by Hartle and Hawking [7]. The former is given by the wave function only consisting of the outgoing mode at the asymptotic future of mini-superspace, and is analogous to the tunneling wave function in quantum mechanics. The latter is given by the path integral over Euclidean non-singular compact geometries with no-boundary. The path integral representation of the wave function provides important notions such as analytic continuation of integration contours, complex action and complex Euclidean solutions called the fuzzy instantons [9, 10]. They play important rolls when we consider semi-classical evaluation of the wave function of the universe based on the saddle point method [11]. A choice of the path integral contour corresponds to specifying a boundary condition of the WD equation [12, 13]. To predict the classical universe using quantum cosmology, we must derive a probability for classical observables from the wave function of the universe. The number of e-foldings of inflation is often used as a predictable observable and recent observational restriction requires this number must be greater than about 60. The amount of e-foldings predicted by quantum cosmology depends on models and boundary conditions. Thus, the main issue in quantum cosmology is to determine which type of boundary conditions are preferable to explain observational results. Recent applications of quantum cosmology to various cosmological models are studied in papers [14–17].

In this paper, we apply a numerical method to obtain predictions from wave functions of

the universe. The main idea of our research is to represent boundary conditions of the wave function using exact solutions of the WD equation with a constant scalar field potential. This makes our problem of determining boundary conditions as the parameter estimation in space of boundary conditions. We aim to obtain a probability distribution of boundary conditions under the constraint of sufficient e-foldings of the inflation. This paper is organized as follows. In section II, we introduce a mini-superspace model and review derivation of the probability for classical universes from the wave function of the universe. In section III, we introduce a parametrization of boundary conditions and define the probability for boundary conditions. Details of our numerical simulations and their results are explained in section IV. Section V is devoted to summary and conclusion. We use the unit in which $c = \hbar = 1$ throughout the paper.

II. MINI-SUPERSPACE MODEL

A. Classical model and quantization

We consider the Einstein gravity with a cosmological constant and a minimally coupled massive scalar field as the inflaton. The action of the gravity is given by

$$S_G = \frac{1}{16\pi G} \int d^4x \sqrt{-g} (R - 2\Lambda), \quad (1)$$

and the action of the scalar field Φ is

$$S_m = -\frac{1}{2} \int d^4x \sqrt{-g} [(\partial_\mu \Phi)^2 + m^2 \Phi^2]. \quad (2)$$

We assume a homogeneous and isotropic closed universe. Then the geometry of the universe is given by the Friedmann-Robertson-Walker (FRW) metric with a scale factor. We assume the following form of the metric:

$$ds^2 = \frac{3}{\Lambda} \left(-\frac{N^2}{q} d\lambda^2 + q d\Omega_3^2 \right), \quad (3)$$

where λ is a dimensionless time parameter and N is a lapse function. We introduce a dimensionless field variable ϕ and its mass μ as

$$\phi = \left(\frac{4\pi G}{3} \right)^{1/2} \Phi, \quad \mu = \left(\frac{3}{\Lambda} \right)^{1/2} m. \quad (4)$$

Then the total action of our model becomes

$$S = \frac{K}{2} \int d\lambda N \left[-\frac{1}{4} \left(\frac{q'}{N} \right)^2 + q^2 \left(\frac{\phi'}{N} \right)^2 + 1 - q(1 + \mu^2 \phi^2) \right], \quad (5)$$

where $' = d/d\lambda$ and we introduced a constant $K \equiv 9\pi/(2G\Lambda)$. In this model, dynamical variables are the scale factor $q(\lambda)$ and the inflaton field $\phi(\lambda)$. We represent them as coordinates of configuration space

$$q^A = (q^0, q^1) = (q, \phi). \quad (6)$$

This configuration space is called mini-superspace. The total Hamiltonian of our mini-superspace model is given by

$$H_T = \frac{KN}{2} \left[\frac{1}{K^2} \left(-4p_q^2 + \frac{1}{q^2} p_\phi^2 \right) - 1 + q(1 + \mu^2 \phi^2) \right] = NH. \quad (7)$$

We obtain the Hamiltonian constraint by taking variation of the lapse function N :

$$H = 0. \quad (8)$$

Canonical quantization of the model is performed by replacing p_A in the Hamiltonian constraint by differential operator \hat{p}_A

$$p_A \rightarrow \hat{p}_A = -i \frac{\partial}{\partial q^A}, \quad (9)$$

and imposing operator version of the Hamiltonian constraint \hat{H} on a physical state $\Psi(q^A)$. It yields the Wheeler-DeWitt equation

$$\left[\frac{1}{2K^2} \left(4 \frac{\partial^2}{\partial q^2} - \frac{1}{q^2} \frac{\partial^2}{\partial \phi^2} \right) - \frac{1}{2} + qV(\phi) \right] \Psi(q, \phi) = 0, \quad V(\phi) \equiv \frac{1}{2} + \frac{\mu^2}{2} \phi^2. \quad (10)$$

In terms of q^A ,

$$\left[-\frac{1}{2K^2} G^{AB} \partial_A \partial_B + U(q) \right] \Psi(q) = 0, \quad U = -\frac{1}{2} + qV, \quad (11)$$

where $G^{AB} = \text{diag}(-4, 1/q^2)$ is a metric of mini-superspace. The wave function $\Psi(q^A)$ on mini-superspace is called the wave function of the universe. Although there is an operator ordering ambiguity in the quantization procedure, we choose the ordering which yields the equation (10) in our analysis.

The wave function Ψ can also be expressed by the path integral with respect to q^A and N :

$$\Psi(q^A) = \int \mathcal{D}N \mathcal{D}q^A e^{iS[N(\lambda), q^A(\lambda)]}, \quad S[N(\lambda), q^A(\lambda)] = \int_0^1 d\lambda \mathcal{L}[N(t), q^A(t)]. \quad (12)$$

Here, $q^A \equiv q^A(1)$ is a boundary value of q^A on the final spacelike hypersurface $\lambda = 1$. The path integral representation of the wave function satisfies Eq. (10) [4]. In our approach to the quantum cosmology, we mainly focus on solving (10) as a differential equation but the path integral representation plays an important roll in characterizing boundary conditions for the wave function.

B. Semi-classical approximation and probability

1. WKB wave function

To extract predictions for the classical universe from the wave function, it must be expressed as the semi-classical form, which means the wave function behaves as the WKB solution of Eq. (10). We perform the WKB expansion of the wave function as

$$\Psi(q^A) = C(q^A) e^{-\frac{1}{\hbar} I(q^A)}. \quad (13)$$

For convergence of the path integral representation of the wave function, the contour of the path integral must be analytically continued in the complex plane. Thus, I and C would generally become complex functions. We write I as $I = I_R - iS$ where I_R and S are real functions. We call $I_R(q^A)$ as a pre-factor and $S(q^A)$ as a phase of the wave function.

Inserting (13) into the WD equation (11), we obtain a set of semi-classical equations for I, C :

$$O(\hbar^0) : \quad -\frac{1}{2K^2}(\nabla I)^2 + U(q^A) = 0, \quad (14)$$

$$O(\hbar^1) : \quad 2\nabla I \cdot \nabla C + C\nabla^2 I = 0, \quad (15)$$

where $(\nabla I)^2 = G^{AB} \partial_A I \partial_B I$, $(\nabla I) \cdot (\nabla C) = G^{AB} \partial_A I \partial_B C$, $\nabla^2 I = G^{AB} \partial_A \partial_B I$. Now, we consider a condition of the wave function to provide predictions for the classical universe. In the classical regime, the phase of the wave function must satisfies the Hamilton-Jacobi equation. This implies that the equation (14) corresponds to the Hamilton-Jacobi equation

in the classical regime. Namely,

$$-\frac{1}{2}(\nabla I_R)^2 + i\nabla I_R \cdot \nabla S + \frac{1}{2}(\nabla S)^2 + K^2 U = 0 \quad (16)$$

should reduce to the classical Hamiltona-Jacobi equation

$$\frac{1}{2K^2}(\nabla S)^2 + U = 0. \quad (17)$$

Thus I_R and S should satisfy the condition

$$\frac{|\nabla I_R|^2}{|\nabla S|^2} \ll 1. \quad (18)$$

This inequality is called the “classicality” condition [10]. To predict the evolution of classical universes from the wave function, I , S and C must satisfy (14)-(18) and we expect that the probability can be obtained in the region of mini-superspace where the classicality condition is satisfied.

In the path integral representation of the wave function, there are more than one saddle point of the action in general. Thus, the semi-classical wave function is given by superposition of WKB components associated with different saddle points:

$$\Psi(q^A) = \sum_{i=\text{saddle}} C^{(i)}(q^A) e^{-I_R^{(i)}(q^A)} e^{iS^{(i)}(q^A)}. \quad (19)$$

It is possible to obtain a desirable probability measure for the classical universe using this expression of the WKB wave function.

2. Conserved current and probability

Now let us consider how to define probability from the wave function. Introducing probability from the wave function of the universe is not straightforward because the WD equation is the Klein-Gordon type and its conserved charge is not positive definite. However, by considering the classicality condition, it is possible to introduce a suitable probability measure and we can define the conditional probability giving predictions for observables. For the wave function Ψ satisfying the WD equation, we have the following conserved current in mini-superspace

$$\mathcal{J}_A = \frac{i}{2}(\Psi^* \nabla_A \Psi - \Psi \nabla_A \Psi^*), \quad \nabla \cdot \mathcal{J}_A = 0. \quad (20)$$

In the classical region where the wave function has the WKB form, we can obtain the positive definite probability measure from \mathcal{J}_A . For each WKB components of the wave function (19), we define

$$J_A^{(i)} \equiv -|C^{(i)}|^2 \exp(-2I_R^{(i)}) \nabla_A S^{(i)}. \quad (21)$$

They are conserved independently in the classical region $\nabla \cdot J^{(i)} = 0$. From the Hamilton-Jacobi equation, we can assign the canonical momentum in the classical region

$$p_A^{(i)} = \nabla_A S^{(i)} = \frac{\partial S^{(i)}}{\partial q^A}. \quad (22)$$

Here, we focus only on the components with $p_q^{(i)} = \partial_q S^{(i)} < 0$. From $dq^{(i)}/d\lambda \propto -p_q^{(i)} > 0$, these components correspond to expanding universes. Thus, we can introduce a conserved current corresponding to expanding universes as

$$J_A^+ \equiv - \sum_{p_q^{(i)} < 0} |C^{(i)}|^2 \exp(-2I_R^{(i)}) \nabla_A S^{(i)}. \quad (23)$$

Let us consider a surface Σ_c in mini-superspace which is spacelike with respect to the metric G_{AB} and has a unit normal n_A . We require the classicality condition (18) is satisfied on this surface. Then the relative probability $\mathcal{P}(\Sigma_c)$ of classical histories passing through this surface is given by the component of the conserved current (23) along the normal if it is positive. In the leading order in \hbar , this is

$$\mathcal{P}(\Sigma_c) \equiv J^+ \cdot n = - \sum_{p_q^{(i)} < 0} |C^{(i)}|^2 \exp(-2I_R^{(i)}) \nabla_n S^{(i)}, \quad (24)$$

where ∇_n means differentiation along the normal vector n_A . As a point on Σ_c is specified by the value of the scalar field, $\mathcal{P}(\phi) \equiv \mathcal{P}(\Sigma_c(\phi))$ provides the probability for the inflaton field to realize a value ϕ on Σ_c .

3. Conditional probability for observables

We can derive a probability for observables from the probability measure $\mathcal{P}(\phi)$. It can be given as the conditional probability [2]

$$P(s_0|s_1) = \frac{\int_{s_0} J \cdot d\Sigma_c}{\int_{s_1} J \cdot d\Sigma_c}, \quad s_0 \subset s_1, \quad (25)$$

where s_1 is a subset of the hypersurface Σ_c defined by some theoretical constraints and s_0 is a subset of s_1 defined by restricting s_1 using observational constraints. By using the relation (22), we can obtain classical trajectories starting from Σ_c . Namely, the probability measure on Σ_c with the classicality condition gives probability distribution of initial data (p_q, q, p_ϕ, ϕ) for the classical equation of motion. In our analysis, the number of e-foldings \mathcal{N} is adopted as an observable because this variable quantifies the inflationary models to explain the horizon and the flatness problems. \mathcal{N} is defined by

$$\mathcal{N} \equiv \log \left(\frac{a(t_f)}{a(t_i)} \right), \quad (26)$$

where t_i denotes the beginning time of inflation and t_f denotes the end time of inflation. In our analysis, we define t_f as the end time of inflation driven by the scalar field potential. The number of e-foldings \mathcal{N} is determined by the initial data and it is possible to translate the probability measure for ϕ on Σ_c to the probability measure for $\mathcal{N}(\phi)$.

To introduce the conditional probability, we define an interval s_1 as $s_1 = [\phi_{\min}, \phi_{\text{pl}}]$ where ϕ_{\min} is the lower bound of the interval and $\phi_{\text{pl}} = 4\sqrt{2K}/(3\mu)$ is the value of the inflaton field corresponding to the Planck energy density m_{pl}^4 . Then an interval $s_0 \subset s_1$ is defined as $s_0 = [\phi_{\text{suf}}, \phi_{\text{pl}}]$ where ϕ_{suf} corresponds to the number of e-foldings $\mathcal{N}_{\text{suf}} \approx 60$ consistent with observations. Accordingly, the conditional probability to predict the universe with sufficient inflation becomes

$$P(s_0|s_1) = \frac{\int_{\phi_{\text{suf}}}^{\phi_{\text{pl}}} d\phi \mathcal{P}(\phi)}{\int_{\phi_{\min}}^{\phi_{\text{pl}}} d\phi \mathcal{P}(\phi)}. \quad (27)$$

We denote this probability as

$$P_{\text{suf}} \equiv P(s_0|s_1) = P(\mathcal{N} \geq 60). \quad (28)$$

The expectation value of \mathcal{N} can be calculated as

$$\langle \mathcal{N} \rangle = \frac{\int_{\phi_{\min}}^{\phi_{\text{pl}}} d\phi \mathcal{N}(\phi) \mathcal{P}(\phi)}{\int_{\phi_{\min}}^{\phi_{\text{pl}}} d\phi \mathcal{P}(\phi)}. \quad (29)$$

These probability and expectation value depend not only on cosmological models but also on boundary conditions of the wave function. As we have already commented in the introduction, there are two well known proposals for the boundary condition of the wave function. One of them is “no-boundary boundary condition proposal” by Hartle and Hawking (HH), the other one is “tunneling proposal” by Vilenkin (V). They predict different evolution of

universe; (HH) prefers small value of \mathcal{N} , on the other hands, (V) prefers large value of \mathcal{N} . By calculating and comparing P_{suf} for given models and given boundary conditions, we can evaluate what type of models and boundary conditions are more suitable to explain observation of our universe.

III. PROBABILITY FOR BOUNDARY CONDITIONS

When we have some restriction on our models of inflationary universe from observations, we can investigate a probability which states preferable type of boundary conditions. It is possible to express this probability using Bayes' theorem:

$$P(B_i|S) = \frac{P(B_i)P(S|B_i)}{\sum_k P(B_k)P(S|B_k)}, \quad (30)$$

where $P(B_i|S)$ is a probability for B_i under S happened. Here, B_i is some candidate of a boundary condition of the wave function labeled by index i , and S means the universe with sufficient inflation, namely, $\mathcal{N} \geq 60$. Thus, $P(B_i|S)$ denotes the probability for B_i under the sufficiently inflated universe. On the contrary, $P(S|B_i)$ in the right hand side is the probability for sufficient inflation under the boundary condition B_i and is equivalent to P_{suf} defined in the previous section

$$P(S|B_i) = P_{\text{suf}}(B_i) = P(\mathcal{N} \geq 60 | B_i). \quad (31)$$

As we do not have any information on the prior probability $P(B_i)$, we assume that it is uniformly distributed. To represent different boundary conditions, we will introduce two parameters a, b in (36). The probability for the parameters a, b is given by

$$P(a, b|S) = \frac{P(S|a, b)}{\int da' db' P(S|a', b')}. \quad (32)$$

When we solve the WD equation, we have to impose some boundary condition (in other words, initial condition) on the wave function. For this purpose, we use exact solutions of the WD equation which are obtained when the scalar field potential $V(\phi)$ is constant. Based on the path integral representation of the wave function, for the constant scalar field potential case, the wave function corresponding to the no-boundary (Hartle-Hawking) and the tunneling (Vilenkin) type boundary conditions are expressed as [12]

$$\Psi_{\text{HH}} = \Psi_2 + \Psi_3, \quad \Psi_{\text{V}} = \Psi_1 + i \Psi_3, \quad (33)$$

TABLE I: Typical wave functions and their parameters (a, b) and asymptotic behaviors. The phase function S_0 is defined by $S_0 = K/(6V)(2qV - 1)^{3/2} - \pi/4$.

wave function	parameter (a, b)	asymptotic form for $q \gg 1$
Ψ_{HH}	$(\pi/4, 0)$	$\sim \exp(+K/(6V)) \cos S_0$
Ψ_V	$(\pi/4, \pi/2)$	$\sim \exp(-K/(6V)) \exp(-iS_0)$
Ψ_1	$(\pi/2, \pi/2)$	$\sim \exp(-K/(6V)) \cos S_0$
Ψ_2	$(\pi/2, 0)$	$\sim \exp(+K/(6V)) \cos S_0$
Ψ_3	$(0, \text{any values})$	$\sim -\exp(-K/(6V)) \sin S_0$

where

$$\Psi_1 \equiv (2V)^{-1/3} \text{Ai}(z_0) \text{Ai}(z), \quad \Psi_2 \equiv (2V)^{-1/3} \text{Bi}(z_0) \text{Ai}(z), \quad \Psi_3 \equiv (2V)^{-1/3} \text{Ai}(z_0) \text{Bi}(z), \quad (34)$$

with

$$z = z(q) = \left(\frac{4V}{K}\right)^{-2/3} (1 - 2qV), \quad z_0 = z(0) = \left(\frac{4V}{K}\right)^{-2/3}. \quad (35)$$

For large values of the scale factor (classical region), Ψ_{HH} is superposition of expanding and contracting universes with amplitude $\exp(+K/(6V))$ which prefers small values of the potential. On the other hand, Ψ_V represents an expanding universe with amplitude $\exp(-K/(6V))$ which prefers large values of the potential. We can express more general type of wave functions introducing two real parameters a, b which represent boundary conditions of the wave function

$$\Psi_C = \tan a (\cos b \Psi_2 - i \sin b \Psi_1) + \Psi_3, \quad 0 \leq a, b \leq \pi/2. \quad (36)$$

Introduced parameters a, b distinguish boundary conditions of the wave function (Table I and Fig. 1). Solving the wave function and calculating probability P_{surf} for different values of (a, b) , we can evaluate the probability for the parameters (a, b) using the relation (32).

IV. NUMERICAL SIMULATION OF THE WAVE FUNCTION

A. Boundary conditions and probability

We solve the WD equation (10) numerically to obtain the probability of boundary conditions. We prepare the initial surface $q = q_{\text{ini}}$ in the Euclidean region of mini-superspace

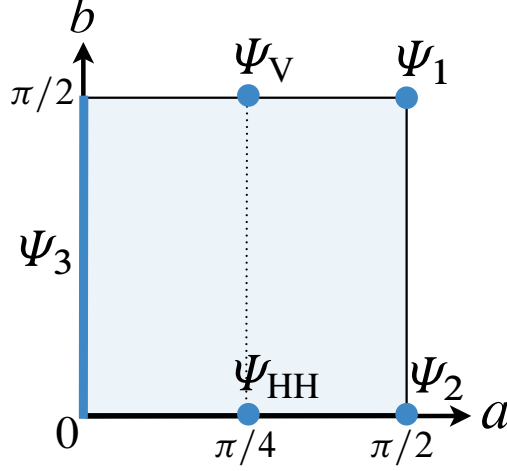


FIG. 1: Parametrization (a, b) of boundary conditions for Ψ_C .

and impose the following boundary condition for the wave function $\Psi(q, \phi)$

$$\Psi(q_{\text{ini}}, \phi) = \Psi_C(q_{\text{ini}}, \phi), \quad \partial_q \Psi(q_{\text{ini}}, \phi) = \partial_q \Psi_C(q_{\text{ini}}, \phi). \quad (37)$$

As Ψ_C introduced by (36) is specified by two parameters (a, b) , this boundary condition is also specified by these two parameters. We call Ψ_C the boundary wave function. For models with a constant scalar field potential, this boundary condition of course reproduces the exact solution Ψ_C .

In the Lorentzian region of mini-superspace with sufficiently large value of ϕ , the WD equation (10) has the following asymptotic form

$$\left[\frac{4}{K^2} \frac{\partial^2}{\partial q^2} - 1 + 2qV(\phi) \right] \Psi(q, \phi) \approx 0, \quad (38)$$

and the exact solution of this equation is given by

$$\Psi_\infty = \alpha_1(\phi) \text{Ai}(z) + \beta_1(\phi) \text{Bi}(z), \quad z(q, \phi) = \left(\frac{4V(\phi)}{K} \right)^{-2/3} (1 - 2qV(\phi)). \quad (39)$$

Using the asymptotic form of the Airy function, Ψ_∞ can be expressed as superposition of two WKB modes corresponding to an expanding universe and a contracting universe

$$\Psi_\infty(q, \phi) \approx C_+(\phi) e^{-iS_0(q, \phi)} + C_-(\phi) e^{iS_0(q, \phi)}, \quad (40)$$

where S_0 is the phase function given by

$$S_0(q, \phi) = \frac{K}{6V(\phi)} (2V(\phi)q - 1)^{3/2} - \frac{\pi}{4}. \quad (41)$$

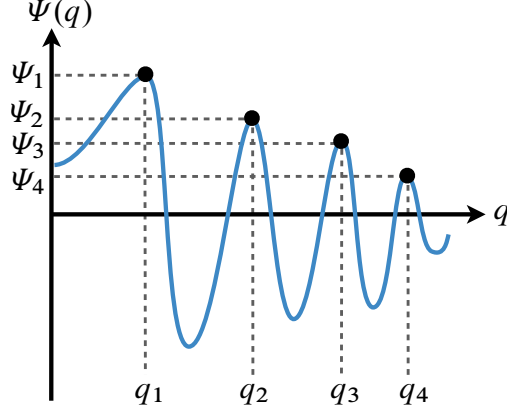


FIG. 2: Local maximum points are determined from the numerical data of the wave function.

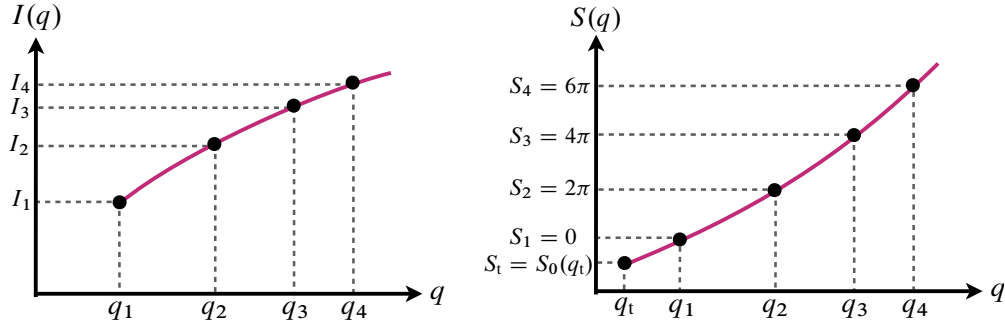


FIG. 3: From the data set $[q_i, \Psi_i]$, the prefactor $I_{R,I}$ and the phase function $S_{R,I}$ are determined by interpolation.

By fitting the numerically obtained wave function Ψ_{num} with Ψ_{∞} , we determine the prefactor of the WKB mode for the wave function Ψ_{num} . Let us denote real and imaginary part of the wave function Ψ_{num} for a fixed value of ϕ as

$$(\Psi_{\text{num}}(q))_R = \exp[-I_R(q)] \cos S_R(q), \quad (\Psi_{\text{num}}(q))_I = \exp[-I_I(q)] \cos S_I(q). \quad (42)$$

From $(\Psi_{\text{num}})_{R,I}$, it is possible to determine locations q_i of local maximum points of the wave function and their values Ψ_i . Thus, we obtain a set of data $[q_i, \Psi_i]$. Then, we obtain $(I(q))_{R,I}$ by interpolation of $(I_i)_{R,I}$ as Fig. 3 (left panel). We can also obtain phase functions $S_{R,I}$ using a reference point $q_t = 1/(2V(\phi))$ with the asymptotic phase function S_0 as Fig. 3 (right panel). Repeating above procedures for other values of ϕ , we can determine a set of functions $(I_{R,I}(q, \phi), S_{R,I}(q, \phi))$ in the Lorentzian region.

Next, we introduce the phase difference relative to $S_0(q, \phi)$ from the numerical data as

$$\varphi_R = S_R - S_0, \quad \varphi_I = S_I - S_0. \quad (43)$$

After that, we evaluate real and imaginary part of WKB amplitudes as

$$C_{R+} = \frac{1}{2}e^{-I_R}e^{-i\varphi_R}, \quad C_{R-} = \frac{1}{2}e^{-I_R}e^{i\varphi_R}, \quad C_{I+} = i\frac{1}{2}e^{-I_I}e^{-i\varphi_I}, \quad C_{I-} = i\frac{1}{2}e^{-I_I}e^{i\varphi_I}. \quad (44)$$

Finally, we obtain amplitudes of the expanding and collapsing mode of the WKB wave function as

$$C_+ = C_{R+} + C_{I+}, \quad C_- = C_{R-} + C_{I-}. \quad (45)$$

The probability measure for the expanding universe is

$$\mathcal{P}(\phi) = -|C_+|^2 \nabla_n S_0, \quad (46)$$

where n denotes a unit normal vector to a specified spacelike hypersurface Σ_c in the classical region of mini-superspace.

To determine the hypersurface on which the probability is defined, we must check the classicality condition (18) in our simulation. The formal definition of the classicality is already introduced in the section II, but applying it directly is not so easy because decomposing the wave function to the phase function and the prefactor is difficult. However, as we also mentioned above, we assume that the phase of the wave function can be well approximated by the asymptotic phase function S_0 in the Lorentzian region. Thus, we can define the desirable classicality condition for our simulation as follows

$$R_c \equiv \sum_{i=R,I} \frac{|(\nabla \tilde{I}_i)^2 + \nabla^2 \tilde{I}_i + i(2\nabla \tilde{I}_i \nabla S_0 - \nabla^2 S_0)|}{|(\nabla S_0)^2|} \ll 1, \quad (47)$$

where \tilde{I}_i is defined by

$$\tilde{I}_{R,I} \equiv I_{R,I} + i\varphi_{R,I}. \quad (48)$$

When we calculate the probability for the classical universe, we should choose a hypersurface Σ_c with $R_c \ll 1$.

B. Simulation set up

We fix the mass of the scalar field and consider two models with parameters $\mu = 0.2$ ($m^2 = 0.03$, $\Lambda = 2.25$) and $\mu = 3$ ($m^2 = 0.03$, $\Lambda = 0.01$). Different value of μ corresponds to different value of the cosmological constant in our analysis. The former choice results in slow roll inflation followed by over damped rolling of the inflaton field and the later results

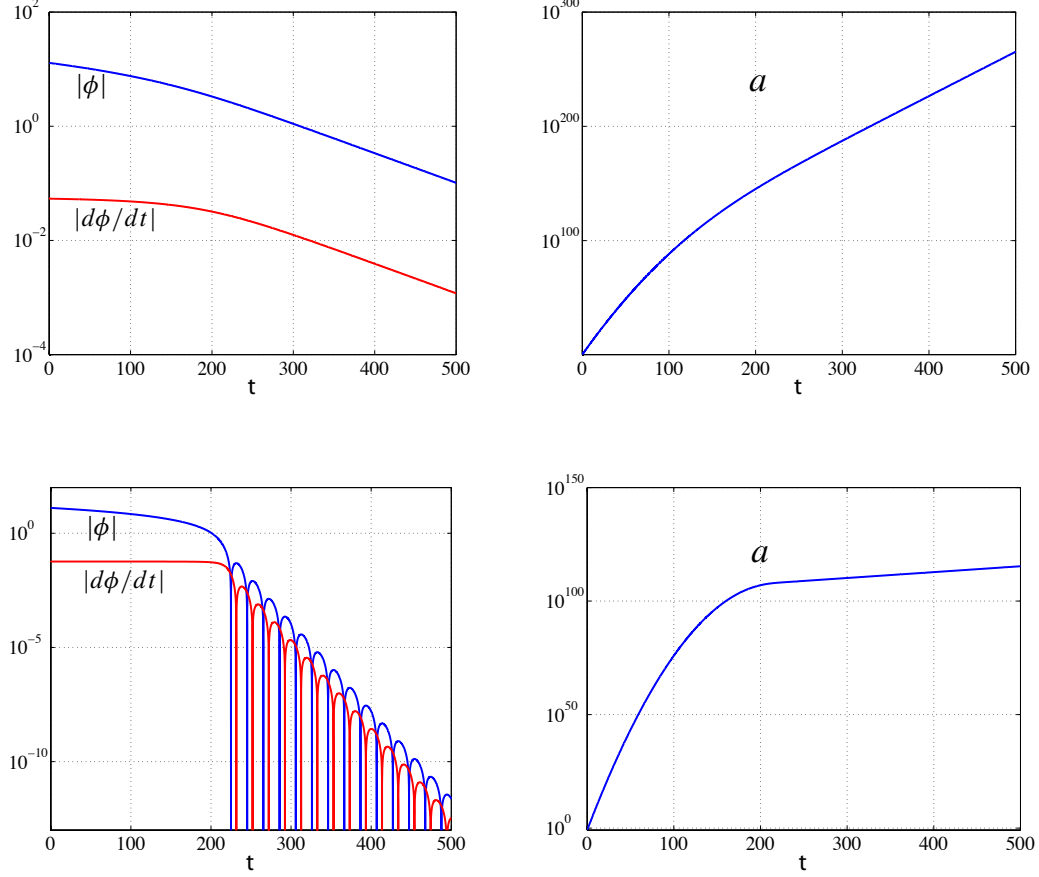


FIG. 4: Classical evolutions of the inflaton $\phi(t)$ and the scale factor $a(t)$ for $\mu = 0.2$ (upper panels) and $\mu = 3$ (lower panels).

in inflation with slow rolling followed by oscillation of the inflaton about $\phi = 0$. Samples of classical trajectory for these models are shown in Fig. 4. The upper panels of Fig. 4 shows a classical evolution of $\mu=0.2$ model in terms of cosmic time t . The inflaton field ϕ and its time derivative $\dot{\phi}$ decay monotonically and inflation do not end (over damped oscillation). Until $t_f \sim 200$ (in the unit of the Planck time), inflation is driven by the mass term potential and after that time, inflation is driven by the cosmological constant. The lower panels of Fig. 4 shows a classical evolution of $\mu = 3$ model. In this model, ϕ decays and then oscillates with exponentially damping at late time. The universe continues accelerated expansion after the slow roll due to the cosmological constant. Two different behavior of classical solutions can be discriminated by the dimensionless parameter μ . For $\mu < \mu_*$, classical trajectories behave like the upper panels (over damped). For $\mu > \mu_*$, classical trajectories behave as the lower panels (oscillation after slow roll). The critical value μ_* determined by our simulation

is $\mu_* \approx 1.5$.

Our simulation algorithm is as follows:

1. Prepare an initial surface $q = q_{\text{ini}}$ in the Euclidean region of mini-superspace close to $q = 0$. q_{ini} cannot be chosen too small because we must keep the Courant condition for stable numerical integration of the wave equation. For the present case, the condition is

$$2q > \frac{\Delta q}{\Delta \phi}, \quad (49)$$

where Δq and $\Delta \phi$ are grid spacings and q_{ini} must satisfy this inequality.

2. Solve the WD equation numerically from $q = q_{\text{ini}}$ to q_{fin} with a given boundary wave function Ψ_C . We adopt the 5-step Adams-Bashforth method for numerical integration which has the 5-th order accuracy. We used 20000×200 grid size which covers $q_{\text{ini}} \leq q \leq q_{\text{fin}}, \phi_{\text{min}} \leq \phi \leq \phi_{\text{max}}$ (actual values used in the simulation is shown in Table II).

TABLE II: Parameters of our simulation.

mass \	K	q_{ini}	q_{fin}	Δq	ϕ_{min}	ϕ_{max}	$\Delta \phi$
$\mu = 0.2$	6.283	0.01	14	6.995×10^{-4}	0	26	0.1307
$\mu = 3$	1413	0.0001	0.2	9.995×10^{-6}	1.8	26	0.1216

3. We specify a hypersurface Σ_c on which the classicality condition (47) is satisfied. We choose Σ_c as a constant S_0 surface. We numerically obtain the probability $\mathcal{P}(\phi)$ on Σ_c .
4. By integrating the classical equation of motion from Σ_c , we evaluate the number of e-foldings for each classical trajectories. Then calculate the probability measure of the e-foldings.
5. Repeating step 2 to step 4 for different values of parameters (a, b) , we obtain the probability of parameters (a, b) which specify boundary conditions of the wave function. We calculate the probability for 9×9 grid points in the parameter space (a, b) of boundary wave functions (Fig. 5).

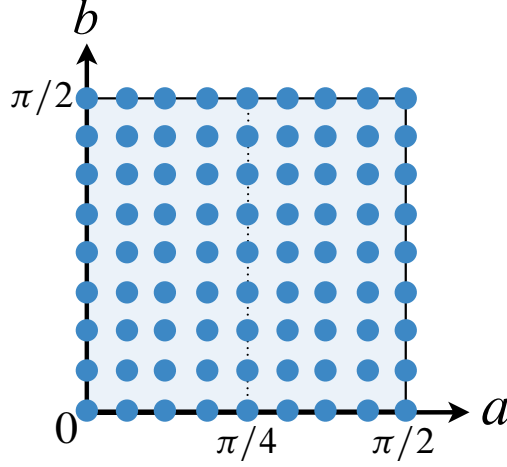


FIG. 5: Parametrization of boundary conditions.

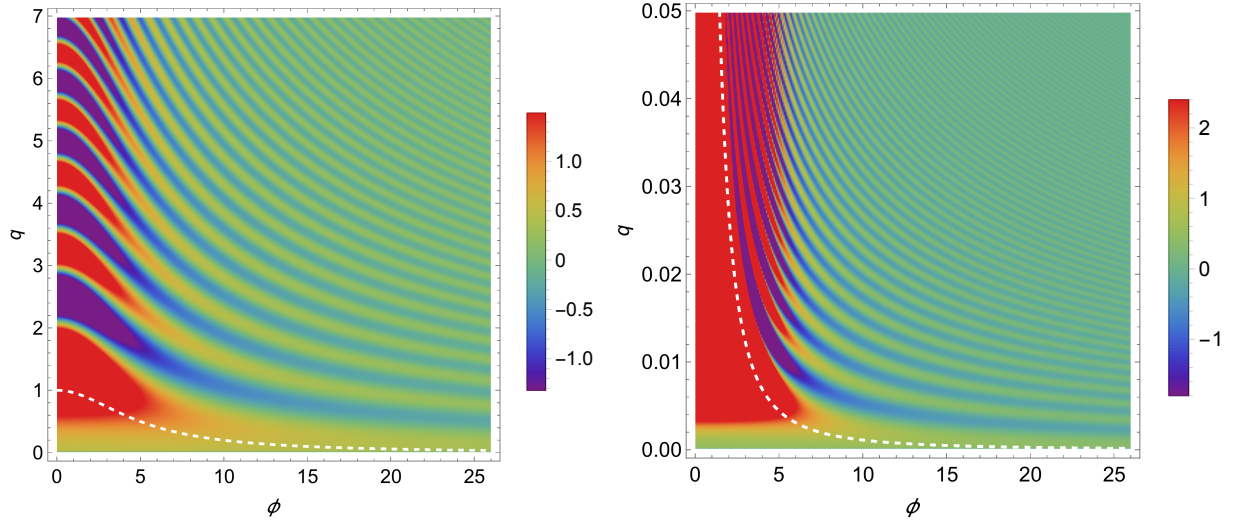


FIG. 6: The density plot of wave functions with the no-boundary boundary condition (HH). Left panel: $\mu = 0.2$ ($m^2 = 0.03$, $\Lambda = 2.25$), $q_{\text{ini}} = 0.01$. Right panel: $\mu = 3$ ($m^2 = 0.03$, $\Lambda = 0.01$), $q_{\text{ini}} = 0.0001$. For this boundary condition, wave functions are real. The dashed line represents $2qV(\phi) = 1$ which is the boundary between the Euclidean region and the Lorentzian region in mini-superspace.

C. Simulation results

Fig. 6 shows wave functions with the boundary wave function Ψ_{HH} (the no-boundary boundary condition (HH)). Fig. 7 and Fig. 8 show wave functions with the boundary wave function Ψ_{V} (the tunneling boundary condition (V)). Fig. 9 shows the classicality condition of the

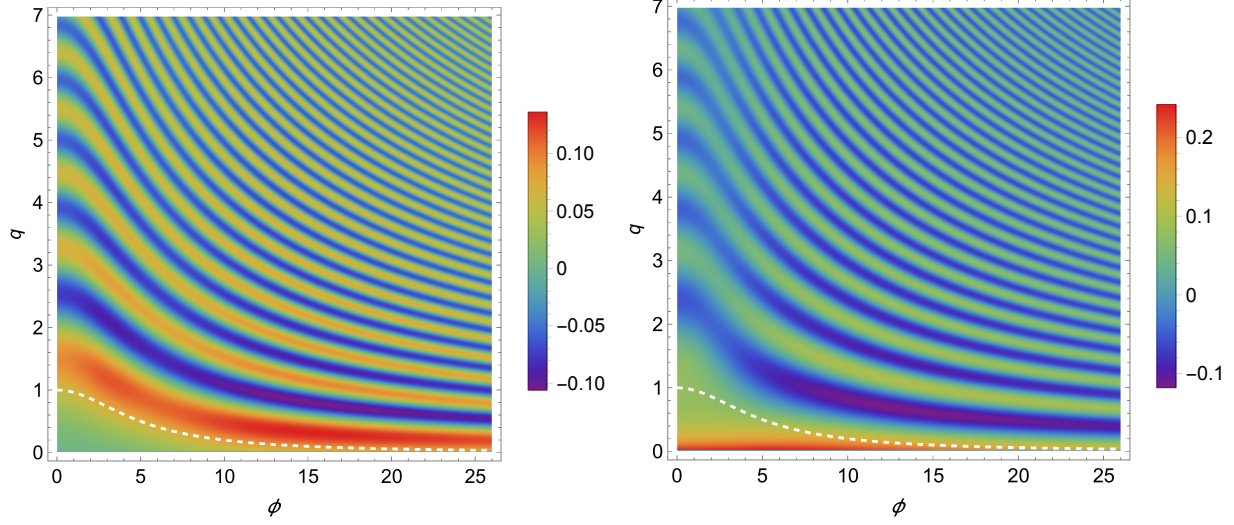


FIG. 7: The density plot of the wave function with the tunneling boundary condition (V) for $\mu = 0.2$, $q_{\text{ini}} = 0.01$ (left: real part, right: imaginary part). The dashed line represents the boundary between the Euclidean region and the Lorentzian region.

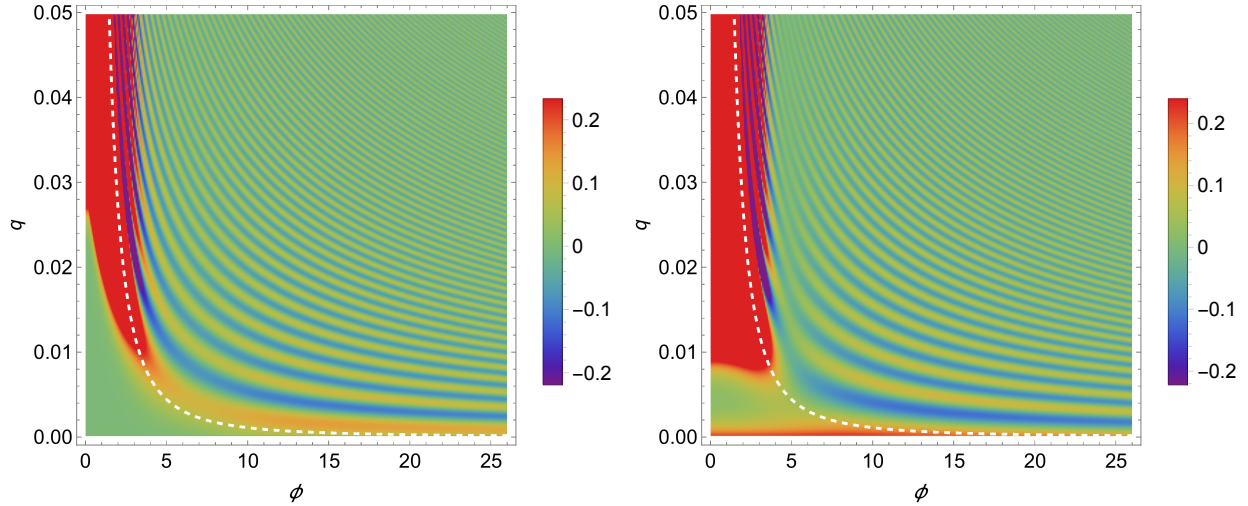


FIG. 8: The density plot of the wave function with the tunneling boundary condition (V) for $\mu = 3$, $q_{\text{ini}} = 0.0001$ (left: real part, right: imaginary part). The dashed line represents the boundary between the Euclidean region and the Lorentzian region.

wave function. We only show the case of the no-boundary boundary condition (HH) because the behavior of the classicality for other wave functions is qualitatively same. We find out the region where the classicality condition is satisfied and define the hypersurface Σ_c in that region. In the case of $\mu = 3$, the classicality condition can not be satisfied for $\phi < 1.8$ and

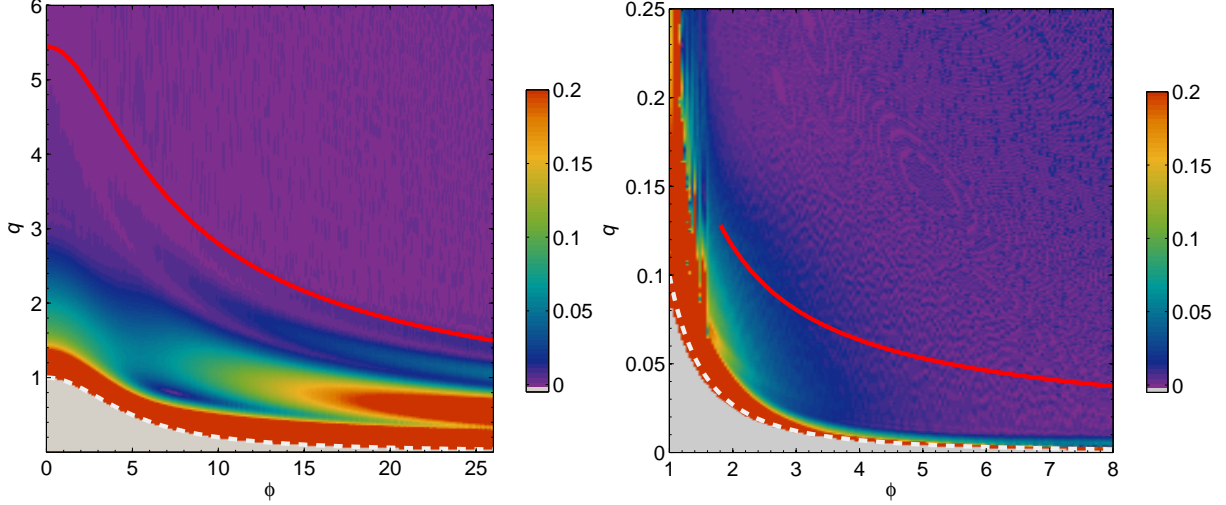


FIG. 9: The density plot of the classicality R_c of the wave function with the no-boundary boundary condition (HH) (left: $\mu = 0.2$, right: $\mu = 3$). Σ_c (solid line) is chosen as $S_0 = \text{const.}$ in the region with $R_c < 0.02$. In the case of $\mu = 3$, the classicality condition can not be satisfied for $\phi < 1.8$. The dashed line represents the boundary between the Euclidean region and the Lorentzian region.

we introduce a cut off ϕ_{\min} to calculate the conditional probability. A similar lower cut off of ϕ is already introduced in [9, 10, 14].

Fig. 10 shows $\mathcal{P}(\phi)$ obtained from solutions of the WD equation obtained with boundary wave functions Ψ_1, Ψ_2, Ψ_3 and Ψ_{HH}, Ψ_V . From now on, we denote wave functions with these boundary wave functions as $\Psi_1, \Psi_2, \Psi_3, \Psi_{\text{HH}}, \Psi_V$. This probability measure is not normalized because the conditional probability $P(S|a, b)$ can be obtained without normalizing $\mathcal{P}(\phi)$. The left panel of Fig. 10 shows $\mathcal{P}(\phi)$ with each boundary conditions for $\mu = 0.2$ model. Wave functions Ψ_1, Ψ_3, Ψ_V prefer large values of ϕ and Ψ_2, Ψ_{HH} prefer small values of ϕ . This behavior of $\mathcal{P}(\phi)$ is the same as that obtained from the exact wave function Ψ_C . However, the distribution for small ϕ is slightly different from that obtained by Ψ_C . A reason for this will be discussed soon later. The right panel of Fig. 10 shows $\mathcal{P}(\phi)$ for $\mu = 3$ model. Probabilities for Ψ_2 and Ψ_{HH} have the same behavior as these in the $\mu = 0.2$ model. However, probabilities for Ψ_1, Ψ_3 and Ψ_V show different behavior; The probabilities for small ϕ have significantly large values for the $\mu = 3$ model.

Here, we explain why behavior of $\mathcal{P}(\phi)$ for three wave functions Ψ_1, Ψ_3 and Ψ_V changes for $\mu = 3$ in the small ϕ region. For $2qV(\phi) \ll 1$, if we assume $V(\phi)$ is constant, the wave function consists of two WKB modes $\Psi_{\pm} \propto \exp(\mp(K/6V)(1 - (1 - 2qV)^{3/2}))$. In this region,

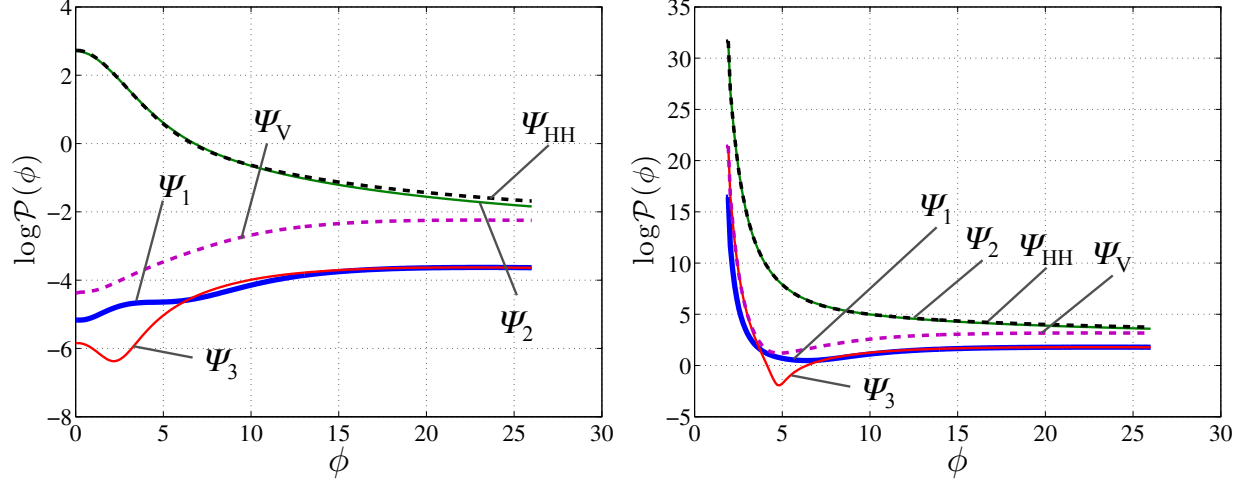


FIG. 10: $\mathcal{P}(\phi)$ for $\mu = 0.2$ (left) and $\mu = 3$ (right). $\mathcal{P}(\phi)$ is not normalized.

the wave functions Ψ_3 and $\text{Im}(\Psi_V)$ are decreasing function of q ($\propto \Psi_-$). On the other hand, the wave functions Ψ_1 and $\text{Re}(\Psi_V)$ are increasing function of q ($\propto \Psi_+$) but their values are kept small due to the prefactor $\exp(-K/(6V))$ (see Table I). The wave function Ψ_3 and $\text{Im}(\Psi_V)$ select the decaying mode and their amplitudes are kept small until reaching the boundary between the Euclidean and the Lorentzian region. However, ϕ dependence of the scalar field potential causes change of the decaying mode Ψ_- to the growing mode Ψ_+ . Ψ_1 and $\text{Re}(\Psi_V)$ contain the growing mode with small amplitudes and contribution of $\partial^2\Psi/\partial\phi^2$ term in the WD equation becomes large around $q \sim q_0$ and enhances amplitudes of their wave functions. As the result, amplitudes of Ψ_1 and $\text{Re}(\Psi_V)$ acquire the similar distribution as Ψ_2 and Ψ_{HH} around the boundary between the Euclidean and the Lorentzian regions. As $\Psi_V = \Psi_1 + i\Psi_3$, all wave functions have the similar distribution except their amplitudes. This behavior of wave functions in the small ϕ region becomes remarkable for large values of the model parameter μ . The mode change and the growth of amplitude explained above may occur for any values of μ (actually, occurs in both cases $\mu = 0.2$ and $\mu = 3$). If μ is small (Λ is large), difference of amplitudes between Ψ_+ and Ψ_- is small and the enhancement of amplitudes of Ψ_1 and $\text{Re}(\Psi_V)$ is not so large. The mode change does not affect behavior of $\mathcal{P}(\phi)$ for small ϕ . But if μ is large (Λ is small), the difference and enhancement of the amplitude of the wave function becomes remarkable and the behavior of $\mathcal{P}(\phi)$ for small ϕ changes.

Using $\mathcal{P}(\phi)$, we obtain the probability measure for number of e-foldings \mathcal{N} by numerical

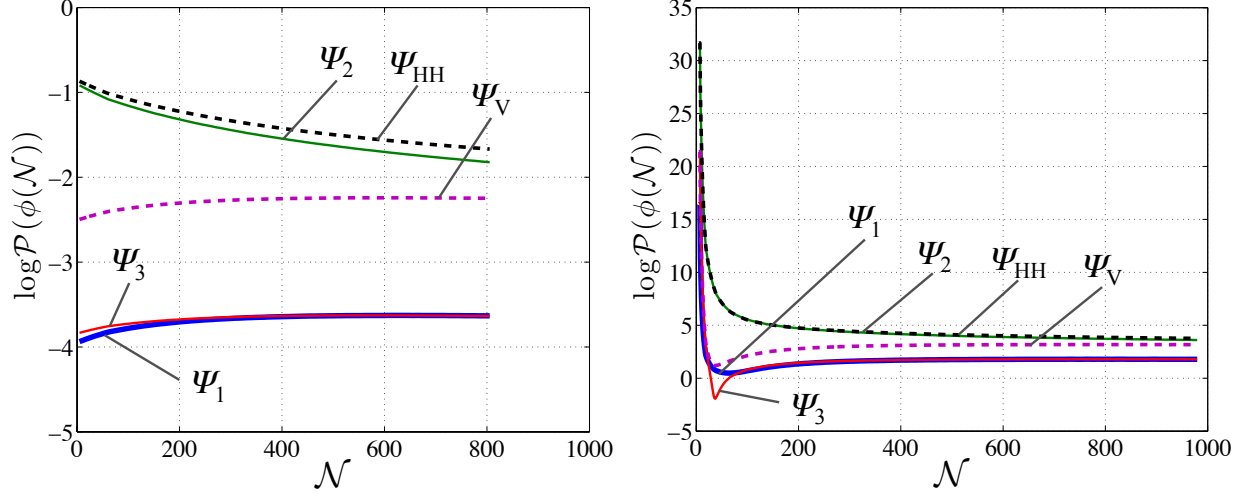


FIG. 11: $\mathcal{P}(\phi(\mathcal{N}))$ for $\mu = 0.2$ (left) and $\mu = 3$ (right). $\mathcal{P}(\phi(\mathcal{N}))$ is not normalized.

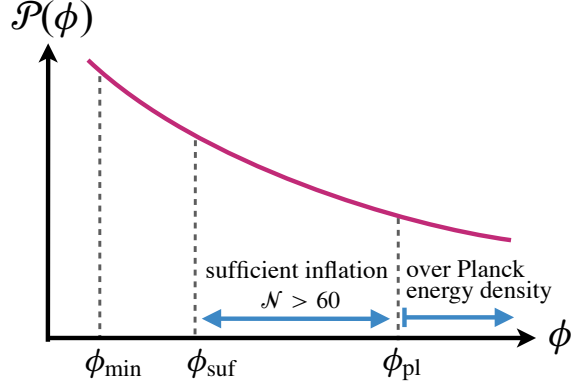


FIG. 12: The probability is defined in $s_0 = [\phi_{\min}, \phi_{\text{pl}}]$. We set $\phi_{\min} = 0$ for $\mu = 0.2$ and $\phi_{\min} = 1.8$ for $\mu = 3$ because the classicality condition is violated in $\phi < 1.8$ region for $\mu = 3$ case.

integrations of classical trajectories starting from Σ_c (Fig. 11). Then, we evaluate the conditional probability for the sufficient inflation $P_{\text{suf}} = P(\mathcal{N} \geq 60)$. The numerical values are shown in Table III, where we consider the probability in the interval $s_0 = [\phi_{\min}, \phi_{\text{pl}}]$ (Fig. 12).

Finally, we obtain the probability $P(a, b)$ of boundary conditions using the relation (32) (Fig. 13).

In the case of $\mu = 0.2$ (left panel of Fig. 13), $P(a, b)$ has large values on lines $a = 0$ and $b = \pi/2$. These two lines correspond to the wave functions Ψ_1 , Ψ_3 and Ψ_V . $P(a, b)$ has small values on the line $b = 0$, corresponding to Ψ_2 and Ψ_{HH} . Consequently, Ψ_V is more preferable than Ψ_{HH} to realize large e-foldings, and this result is the same as one predicted by the wave functions for a constant scalar field potential. In contrast to that, in the case of $\mu = 3$ (right

TABLE III: $P_{\text{suf}} = P(\mathcal{N} \geq 60)$ for five wave functions and two choices of μ . The larger value of P_{suf} is more preferred for sufficient inflation.

mass\wave function	Ψ_1	Ψ_2	Ψ_3	Ψ_{HH}	Ψ_{V}
$\mu = 0.2$	0.604	0.0512	0.627	0.0561	0.621
$\mu = 3$	2.40×10^{-5}	1.60×10^{-10}	1.72×10^{-7}	1.61×10^{-10}	6.74×10^{-7}

TABLE IV: Expectation value of number of e-foldings $\langle \mathcal{N} \rangle$ for five wave functions and two choices of μ . This quantity represents amount of inflation for the classical universe.

mass\wave function	Ψ_1	Ψ_2	Ψ_3	Ψ_{HH}	Ψ_{V}
$\mu = 0.2$	211	15.9	217	17.6	216
$\mu = 3$	6.75	6.74	6.74	6.74	6.74

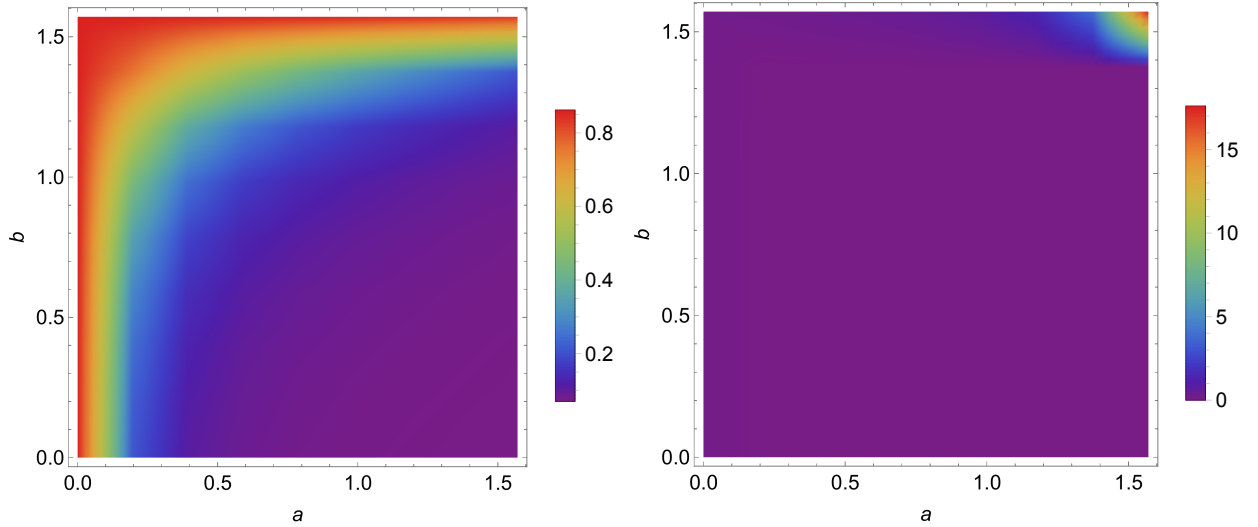


FIG. 13: Density plot of $P(a, b)$ for $\mu = 0.2$ (left) and $\mu = 3$ (right). We evaluated this probability on 9×9 grid points in the parameter space of boundary conditions.

TABLE V: $P(a, b)$ for five wave functions and two choices of μ .

mass\wave function	Ψ_1	Ψ_2	Ψ_3	Ψ_{HH}	Ψ_{V}
$\mu = 0.2$	0.83	0.071	0.86	0.077	0.85
$\mu = 3$	18	1.2×10^{-4}	0.13	1.2×10^{-4}	0.49

panel of Fig. 13), $P(a, b)$ has large values only around the point $(a, b) = (\pi/2, \pi/2)$, which corresponds to the boundary wave function Ψ_1 . This behavior is significantly different from the case of $\mu = 0.2$ (see Table V). Superiority of Ψ_V to Ψ_{HH} holds both $\mu = 0.2$ and $\mu = 3$ models. We expect our results with parameter $\mu = 0.2$ and $\mu = 3$ are typical ones and $P(a, b)$ with $\mu < \mu_*$ behaves similar to $\mu = 0.2$ case and $P(a, b)$ with $\mu > \mu_*$ behaves similar to $\mu = 3$ case.

V. SUMMARY AND CONCLUSION

In this paper, we considered boundary conditions for the wave function of the universe which lead to sufficient e-foldings of inflation. For this purpose, we adopted the exact solutions of the WD equation with a constant scalar field potential as the boundary condition of the wave function, and solved the WD equation numerically. This boundary condition is parametrized with two real parameters and includes both the tunneling and the no-boundary boundary conditions. We obtained the probability distribution function for these parameters under the condition of sufficient e-foldings of inflation. The parameters with large value of this probability determines the boundary condition of the wave function which predicts sufficient e-foldings of inflation. We found that the probability distribution of boundary conditions has two different behavior depending on the value of model parameter μ .

For small values of μ , the cosmological constant dominates and the inflaton field asymptotically approaches to zero without oscillation. In this case, ϕ dependence of the wave function is not so strong and the obtained wave function reproduces behavior of exact wave functions with a constant scalar field potential. Hence the probability of boundary conditions has large values for Ψ_1, Ψ_3, Ψ_V and small values for Ψ_2, Ψ_{HH} . Thus, boundary conditions Ψ_1, Ψ_3, Ψ_V are preferable to realize sufficient period of inflation and superiority among them is small. This behavior of the probability of boundary conditions can be expected from behavior of wave functions for a constant scalar field potential. On the other hand, for large values of μ , the slow roll inflation is followed by oscillation of the inflaton field. In this case, the derivative term of ϕ in the WD equation cannot be neglected and wave functions have large values about $\phi = 0$ for any boundary conditions. Owing to this behavior of the wave function, the probability of boundary conditions has large value about Ψ_1 (superiority of Ψ_V over Ψ_{HH} is kept as before). Thus, realistic inflationary models followed by oscillation

of inflaton field select the boundary condition Ψ_1 .

As an extension of analysis presented in this paper, it is also possible to discuss probability for values of the model parameter μ . The probability distribution of boundary conditions has a sharp peak for the model with large μ and selects a specific boundary condition. This implies that a suitable boundary condition is automatically chosen for large values of μ (small values of the cosmological constant). If we assume that the probability of boundary conditions select an unique boundary condition, the parameter μ must acquire large value (the cosmological constant must be small). To confirm this expectation, we should analyse behaviour of the probability of boundary conditions for wider range of the parameter μ and we will report on this subject in a separate publication.

Acknowledgments

We would like to thank Meguru Komada for introducing us basic concept of Bayesian inference. YN was supported in part by JSPS KAKENHI Grant Number 15K05073 and 16H01094.

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Appendix A: Classical solution

From the Hamiltonian (7), equations of motion for ϕ and q are

$$\frac{1}{N} \left(q^2 \frac{\phi'}{N} \right)' + \mu^2 q \phi = 0, \quad (\text{A1})$$

$$\frac{1}{N} \left(\frac{q'}{N} \right)' = -4q \left(\frac{\phi'}{N} \right)^2 + 2(1 + \mu^2 \phi^2), \quad (\text{A2})$$

$$\frac{1}{4} \left(\frac{q'}{N} \right)^2 = q^2 \left(\frac{\phi'}{N} \right)^2 - 1 + q(1 + \mu^2 \phi^2). \quad (\text{A3})$$

By taking cosmic time t as a time parameter and using the scale factor $a = q^{1/2}$ and the original constants, (A1) and (A3) become

$$\ddot{\Phi} + 3 \left(\frac{\dot{a}}{a} \right) \dot{\Phi} + m^2 \Phi = 0, \quad (\text{A4})$$

$$\left(\frac{\dot{a}}{a} \right)^2 + \frac{\Lambda}{3a^2} = \frac{\Lambda}{3} + \frac{4\pi G}{3} (\dot{\Phi}^2 + m^2 \Phi^2), \quad (\text{A5})$$

where $\dot{} = \frac{d}{dt}$.

Now we consider the solution of slow roll inflation driven by the mass term in this model. The the slow roll condition is

$$|\ddot{\Phi}| \lesssim \left(\frac{\dot{a}}{a} \right) |\dot{\Phi}|, \quad \dot{\Phi}^2 \lesssim m^2 \Phi^2, \quad \frac{\Lambda}{3} \lesssim \frac{4\pi G}{3} m^2 \Phi^2, \quad (\text{A6})$$

and we also assume that the spatial curvature is negligible. Then the scalar field evolves as

$$\Phi \approx \Phi_i - \frac{m}{2\sqrt{3\pi G}} (t - t_i). \quad (\text{A7})$$

The domination of the mass term ends at Φ_f , which depends on the value of a dimensionless parameter $\mu = m/\sqrt{\Lambda/3}$. For $\mu < 3$,

$$\Phi_f \approx \sqrt{\frac{\Lambda}{4\pi G m^2}}, \quad \phi_f = \frac{1}{\mu}, \quad (\text{A8})$$

and below this value, the scalar field evolves as

$$\Phi \approx \Phi_f \exp \left[-\frac{\mu^2}{3} \sqrt{\frac{\Lambda}{3}} (t - t_f) \right]. \quad (\text{A9})$$

The e-foldings from Φ_i to Φ_f is

$$\mathcal{N} = \ln \left(\frac{a_f}{a_i} \right) \approx \frac{3}{2} \left(\phi_i^2 - \frac{1}{\mu^2} \right). \quad (\text{A10})$$

For $\mu > 3$,

$$\Phi_f \approx \frac{1}{2\sqrt{3\pi G}}, \quad \phi_f = \frac{1}{3}, \quad (\text{A11})$$

and below this value, the scalar field oscillates around $\Phi = 0$. The e-foldings from Φ_i to Φ_f is

$$\mathcal{N} = \ln \left(\frac{a_f}{a_i} \right) \approx 2\pi G (\Phi_i^2 - \Phi_f^2) = \frac{3}{2} \left(\phi_i^2 - \frac{1}{9} \right). \quad (\text{A12})$$

The value of the scalar field at the Planck energy is defined by¹

$$\frac{m^2}{2}\Phi_{\text{pl}}^2 = m_{\text{pl}}^4, \quad \phi_{\text{pl}} = \frac{4}{3} \frac{\sqrt{2K}}{\mu}. \quad (\text{A13})$$

As $\phi_{\text{f}} < \phi_{\text{pl}}$, we have the following constraint for parameters in our model

$$\mu < 3 : \quad \frac{9}{32} < K, \quad (\text{A14})$$

$$\mu > 3 : \quad \frac{9}{32} < \frac{\mu^2}{32} < K. \quad (\text{A15})$$

¹ The Planck mass is defined by $m_{\text{pl}}^2 = 1/G$.